REMARKS

This Amendment accompanies a Request for Continued Examination. Entry of the Amendment is respectfully requested before further consideration of the application. Claims 1, 9, and 13-35 were pending. All claims were rejected for the reasons set forth in more detail below. We have amended claims 1, 9, 28, and 35. No claims have been cancelled, added or withdrawn in the Amendment. Claims 1, 9, and 13-35 are pending. We respectfully request reconsideration.

Request for specific citation

The Examiner requested we provide a specific reference to the location in Inventor Helson's review article where Dr. Helson includes symmetry as a "future advance" for structure diagram generation. See Office Action at pg. 10. In Helson, "Structure Diagram Generation", *Reviews in Computational Chemistry*, Vol. 13, Ch. 6, pp. 313-398 (Cite No. CQ in the IDS dated November 4, 2008), Dr. Helson discusses several future advances for structure diagram generation beginning on page 388. Dr. Helson discusses the need to include consideration of symmetry in structural diagram generation on pages 390-91.

The book *Reviews in Computational Chemistry* was first published May 19, 1999. The present application was filed February 11, 2000, and is entitled to the benefit of U.S. Provisional Application No. 60/119,654, filed February 11, 1999.

Rejections under 35 U.S.C. § 103(a)

Claims 1, 9, and 13-35 were rejected under 35 U.S.C. § 103(a) as being obvious over Helson, "Simulation of Carbene Chemistry and Other Problems in Computer-Assisted Organic Synthesis", Purdue University 1993 (herein Helson) in view of Benecke, C., *et al.*, "MOLGEN+, a generator of connectivity isomers and stereoisomers for molecular structure elucidation",

Analytica Chimica Acta, Vol. 314, pp. 141-147, 1995 (herein Benecke). See Office Action at pg. 2. Specifically, the Office Action states that Helson teaches indentifying an instance of chemical structural symmetry and positioning atoms and bonds in a chemical structure diagram. See Office Action at pgs. 2-3. The Office Action also states, however, that Helson does not disclose laying out atoms/bonds to express an identified symmetry. The Office Action relies on Benecke to provide this missing element, stating that Benecke "discloses laying out atoms/bonds to express the identified symmetry". See Office action at pg. 6.

Perception of Stereochemistry Differs from Structure Diagram Generation

Before addressing the specific assertions in the rejection, we provide the following remarks in an attempt to clarify the relationship between the perception of stereochemistry and the process of structure diagram generation.

Simply put, stereochemical perception is a distinct and separate task from structure diagram generation. Stereochemical perception is the process of identifying the relative spatial arrangement of atoms within molecules. Stereochemical perception is not concerned with the visual presentation of a molecular structure. Meanwhile, structure diagram generation is the process by which two-dimensional coordinates for atoms and bonds in a molecule are generated from a connection table to provide a stylized two-dimensional depiction of the chemical structure that can be displayed or printed.

Symmetry is consulted to determine if stereochemistry exists at an atom or bond. For example, if two substituents are symmetrically equivalent, then stereochemistry is said not to exist because a mirror image would be identical to the original. Also, when seeking to generate all molecular graphs that correspond to a given chemical formula, symmetry can be used to eliminate redundancies in the results. However, none of these considerations of symmetry have

anything to do with determining two-dimensional coordinates for atoms and bonds for the purpose of producing a visual representation of a chemical structure corresponding to the given chemical formula.

Said another way, starting with a chemical formula only, and producing one or a set of visual presentations of what molecules the chemical formula could represent involves at least two distinct phases. The first phase is the generation of connection tables, which describe the connectivity of the atoms. Symmetry can be ignored during this phase, and a legitimate set of connection tables would still result. However, to eliminate redundancy in the sets of connection tables, symmetry is often employed to prevent the generation of (or eliminate) connection tables that describe the same molecule.

The second phase is the rendering of the information in the connection tables in a visual format. Regardless of whether symmetry was employed in the generation of the connection tables, the connection tables contain no information as to how symmetrically equivalent atoms and bonds are laid-out to visually express the symmetry.

> *Neither Helson, nor Benecke, alone or in combination, teach or suggest laying out symmetrically equivalent atoms and bonds in a chemical structure diagram to visually express identified symmetry in a stylized two-dimensional pictorial representation of the chemical structure.*

As mentioned above, the Examiner states that Helson does not disclose laying out atoms/bonds to express an identified symmetry. We agree. Moreover, we wish to emphasize that the portions of Helson cited by the Examiner, at most, are concerned solely with the perception of symmetry. Specifically, the AeF-Redraw algorithm, indicated by the Office Action as involving symmetry, simply "assess how well a molecule or collection of molecules

has been drawn." See Helson at pg. 201. Furthermore, Algorithm 3.1 reproduced by the Examiner on page 4 of the Office Action, does not use symmetry or the perception of symmetry for structure diagram generation; nowhere in the description of this algorithm is symmetry discussed. See Helson at pgs. 148-156. For further clarification on the disclosure of Helson, we respectfully refer the Examiner to the amendment filed on July 25, 2008, attached hereto as Exhibit I for the convenience of the Examiner.

We disagree that Benecke discloses laying out atoms/bonds to visually express identified symmetry in a stylized two-dimensional pictorial representation of the chemical structure. Thus, as the combination recited in the rejection does not teach or suggest all elements of amended claim 1, we submit claim 1 is patentable over the cited references.

Benecke describes a structure generator software application, MOLGEN+, which produces all of the molecular graphs that correspond to a given chemical formula. As disclosed in Benecke, MOLGEN+ takes as its input a chemical formula, (optionally) prescribed and forbidden substructures, an interval for allowed ring sizes, and maximal bond multiplicities. From this input, MOLGEN+ generates a complete list of all mathematically possible molecular graphs that are compatible with the chemical formula. After generation of the constitutional isomers, MOLGEN+ produces a sketch of the molecules in the form of a tapestry of several molecules shown together or as a single molecule. See Benecke at pg. 142-44.

However, the MOLGEN+ program does not, nor does Benecke disclose, laying out symmetrically equivalent atoms and bonds in a chemical structure diagram to visually express the identified symmetry in a stylized two-dimensional pictorial representation of the chemical structure, as required by the claimed invention. Benecke only mentions symmetry in connection with what we described above as the "first phase" of the overall process producing a visual

representation of a chemical structure. Specifically, the MOLGEN+ program generates a series of connection tables, which it terms "molecular graphs", that satisfy certain constraints provided by the user, such as the number of atoms present and the valency of the atoms. See Benecke at pgs. 142-143. Next, the MOLGEN+ program uses symmetry to remove redundant candidates from the series of connection tables only. See Benecke at pg. 145 (Benecke states "MOLGEN+ is capable of generating all possible configurational isomers, again redundancy free (which also implies the consideration of symmetries)."). These connection tables, a.k.a. molecular graphs, do not include any information regarding the two-dimensional positioning of atoms and bonds in a stylized pictorial representation of the chemical structure. Again, as set forth above, the actual positioning of atoms and bonds in two-dimensions is a separate phase of the entire process.

Evidence that one having ordinary skill in the art and reading Benecke would conclude that MOLGEN+ merely considered symmetries to avoid duplications when generating all permutations of a list of elements is provided by the Rule 132 declaration of Dr. Harold Helson (herein Declaration). Moreover, as set forth in the Declaration, one having skill in the art would not understand Benecke as disclosing or suggesting the laying out of symmetrically equivalent atoms and bonds in a chemical structure diagram to visually express the identified symmetry in a pictorial representation of a chemical structure.

The Office Action alleges our previous attempt to clarify the role of symmetry in the Benecke approach was "a piecemeal analysis of the combination". See Office Action at pg. 9. We disagree because in that response, we explained why the references alone, and in combination, did not teach or suggest all elements of claim 1. Specifically, as we explained above, combining Benecke's use of symmetry with Helson's positioning of atoms and bonds does not result in the claimed limitation. Again, this is so because Benecke's use of symmetry is

not for relative placement of atoms or bonds in a two-dimensional pictorial representation of a chemical structure.

The Office Action also points to page 145 in Benecke, where the authors state, "In the second step spatial realizations of these isomers are calculated by the application of appropriate geometrical transformations to the placement computed above." See Office Action at pg. 9 (emphasis added in the Office Action). The Examiner then states, "Note fig. 2. Whether this constitutes a 'structure diagram' or not is irrelevant." We are not certain of what significance this portion of Benecke is to the Examiner, nor the meaning of the Examiner's comment, because no further elaboration is provided in the Office Action. If our comments that follow indicate we have misunderstood, we respectfully request the Examiner contact the undersigned to aid our comprehension.

If the Examiner is suggesting this statement in Benecke teaches or suggests the placement of atoms and bonds to visually express symmetry in any way, we respectfully disagree and submit the statement is completely silent regarding symmetry. Moreover, Benecke describes the use of "appropriate geometrical transformations" to calculate spatial realizations of the isomers determined to correspond to a single gross formula. We submit this is no more than the application of molecular mechanics to model, in three-dimensions, the various molecular systems represented by the connection tables generated earlier in the process.

The Office Action states, "It is noted that removal of the 'redundancy' appears to be a natural by-product of identifying and expressing the symmetries, as claimed and as disclosed in the specification." See Office Action at pg. 9. We agree that removal of redundancy is a natural by-product of identifying symmetry. The same is not true of expressing symmetry alone, because, as explained above, building connection tables is completely separate from laying out

atoms and bonds in a pictorial representation of a chemical structure. For example, redundancy could instead be ignored when generating a set of connection tables. Each connection table of the set could then be used to derive a chemical structure diagram in which symmetry is identified and expressed in accordance with the method of claim 1. This would result in a set of pictorial representations expressing any identified symmetries. However, some of the pictorial representations would be identical because redundancies were not removed during the connection table generation process. Thus, we submit that removal of redundancy is discrete from creating a picture expressing symmetry.

The Office Action states, "It is noted that *laying out the symmetrically equivalent atoms and bonds* by itself means that the symmetries are expressed." See Office Action at pg. 11. We strongly disagree because merely depicting a chemical structure that has symmetrically equivalent atoms and bonds does not guarantee that the symmetry is expressed. Figures 3 and 4 of the Application, and the accompanying description, provide clear examples of this distinction. Moreover, we remind the Examiner that he agreed with this position in his Notice of Allowance and Examiner Interview Summary dated October 7, 2008. Specifically, the Examiner stated:

> "The following is a statement of reasons for the indication of allowable subject matter: the prior art of record, while disclosing perception of symmetry, does not disclose expressing the identified symmetry, as expressly claimed in the context of the claims, as disclosed in the specification, and in view of Applicant's remarks on pp. 6-9 of their response."

See Notice of Allowance, dated October 7, 2008, at pg. 2 (emphasis added).

As mentioned above, the entire substance of our amendment filed on July 25, 2008, is attached hereto as Exhibit I for the convenience of the Examiner.

Thus, we submit claim 1 is not obvious over Helson in view of Benecke. Claims 9, 28, and 35 have comparable limitations to those of claim 1, and claims 13-27 and 29-34 depend from

one of claim 1 or 28. Accordingly, we submit these claims are not obvious in view of the cited references for at least the same reasons given for claim 1.

Conclusion

In view of the foregoing remarks, we submit the pending application is in condition for allowance, which action is respectfully requested. If the Examiner believes that a telephone conference would expedite prosecution, the Examiner is asked to contact the undersigned.

This Amendment accompanies a Request for Continued Examination, a Petition for a Three Month Extension of Time, and authorization to charge the fees associated therewith. Please charge any other fees that may be due, or credit any overpayments to our Deposit Account No. 08-0219, under Order No. 0103544.00131US2 from which the undersigned is authorized to draw.

Respectfully submitted,

Dated: March 2, 2010

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